Eulerian modeling and computational fluid dynamics simulation of mono and polydisperse fluidized suspensions

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1 Abstract

Fluidization, the operation consisting in passing a fluid upwards through a bed of particles so as to confer the latter a fluid-like behavior, is a winning technology used in several industrial processes. Designing fluidized bed, however, has always been extremely complex, since the behavior of these systems is difficult to predict. Computational fluid dynamics (CFD) permits to investigate fluidized beds without having to resort to pilot plants and scaling-up empirical relations; it is nonetheless critical that the fluid dynamic models be sufficiently accurate. There are essentially two approaches to model multiphase systems: the *Eulerian-Lagrangian*, which tracks the motion of each particle and solves the dynamics of the fluid at a length scale much smaller than the particle diameter (microscopic length scale), and the *Eulerian-Eulerian* models, based on averaged equations of motion which treat the fluid and solid phases as interpenetrating continua. Being computationally less demanding, this second approach is often preferred, especially by the industry. Its major drawback, however, is that the equations of motion are not mathematically closed and appropriate constitutive relations must be developed on semitheoretical grounds.

My PhD was primarily concerned with the Eulerian-Eulerian mathematical modeling of fluidized suspensions. I started it by deriving rigorously the space-averaged equations of motion for particulate systems of n particle classes (Owoyemi et al., 2007; Mazzei, 2008); this provides considerable insight into the mathematical origin of the various contributions featuring in said equations and is necessary to attain a well-posed multiphase model.

I then developed constitutive relations required to close the fluid-particle interaction force, with particular emphasis on two contributions: the buoyancy force and the drag force.

First, I examined the buoyancy force, comparing the classical definition, which regards it as equal to the weight of fluid displaced by the particles, to alternative definitions used in multiphase flows. I also explained why the classical definition should be preferred (Mazzei & Lettieri, 2007).

Then, I analyzed critically several closure relationships available in the literature used to model the drag force in monodisperse systems (Mazzei & Lettieri, 2007, 2008). To put the validity of these closures to the test, I studied the expansion profiles of homogeneous fluidized beds both analytically and computationally, and I compared the results with experimental data. The analysis showed that no relationship is entirely consistent with the empirical correlation of Richardson & Zaki (1954); in fact, in some fluid dynamic regimes and for some values of the voidage, the predictions were quite at variance. Since this correlation is particularly reliable and accurate, I developed and tested a new equation of closure entirely based on it (Mazzei & Lettieri, 2007); consistency was thus obtained over the whole range of fluid dynamic regimes and for any value of the fluid volume fraction. This property is essential when simulating the motion of fluidized suspensions as it ensures a more accurate prediction of the expansion profiles of homogeneous systems, a feature that indirectly reflects a better assessment of the drag force magnitude.

Successively, I investigated the stability of particulate fluidized systems; this was done analytically by means of linear stability analysis (Mazzei et al., 2006). I observed that if the only fluid-particle interaction forces at play are the buoyancy and the drag, formal stability is not possible – the same conclusion holds if additional terms, such as the virtual mass force or the lift force, are considered. This seems to contradict experimental evidence. To overcome this inconsistency, following Foscolo & Gibilaro (1987), I introduced a novel force, named *elastic force*. Its origin is based on purely physical considerations and is related to void fraction gradients arising when the system homogeneity is lost. The closure that I advanced, as opposed to that developed by the aforementioned authors, is

not limited to conditions approaching equilibrium and holds in a much more general framework, a property which renders it suitable for the CFD study of multiphase flows.

By putting together these results, I proposed a new Eulerian-Eulerian fluid dynamic model for fluidized suspensions that features novel formulations for all the main contributors to the fluid-particle interaction force (Mazzei & Lettieri, 2008).

The model just described caters for monodisperse systems. As previously pointed out, however, an important property of multiphase particulate systems is the particle size distribution of the granular material making up the suspension. To improve the modeling, we must therefore treat the system as polydispersed, considering the presence of several discontinuous phases interacting with one another and with the fluid. To this end, I adopted a more powerful modeling approach to derive suitable equations of change for the disperse phases (Mazzei, 2008). To describe their evolution, I resorted to the generalized population balance equation (GPBE): a continuity statement written in terms of particle velocity and additional coordinates, such as the particle diameter.

Finding the solution of GPBEs usually requires a detailed description of the fluid dynamics and of the interactions between mixing and chemical reactions (if present); for this reason, CFD has become a standard tool for modeling this type of systems. Solving GPBEs within CFD codes is a very interesting and difficult subject, and in recent years many approaches have been considered. The main difficulty resides in the dimensionality of the equation: whereas classical transport equations are three-dimensional, the GPBE is usually written in a higher-dimensional space and consequently is incompatible with customary (*i.e.*, three-dimensional) computational schemes. To solve the equation, I used the *method of moments* (MOM). This requires the use of a limited number of moments of the GPBE to derive three-dimensional transport equations. The limited set of equations, which replaces the single multidimensional population balance equation, keeps the problem tractable when applied to complicated applications in multiphase flows. The main obstacle to the method is that the moment transport equations are mathematically unclosed.

To overcome the problem, I employed two very efficient methods, the *direct quadrature method of moments* (DQMOM) and the *quadrature method of moments* (QMOM). Both approximate the volume density function (VDF) featuring in the GPBE by using a quadrature formula. The methods are very flexible: the number of nodes in the quadrature corresponds to the number of disperse phases simulated. The more the nodes, the better the quadrature approximation; more nodes, however, entail also more complexity and more computational effort. For monovariate systems, *i.e.*, systems with only one internal coordinate in the generalized sense, the methods are entirely equivalent from a theoretical standpoint; computationally, however, they differ substantially.

To conclude my PhD, I used DQMOM to simulate the dynamics of two polydisperse powders initially arranged as two superposed, segregated packed systems (Mazzei, 2008). As fluidization occurs, the simulation tracks the evolution in time and physical space of the quadrature nodes and weights and predicts the degree of mixing attained by the system. To validate the method, I compared computational predictions with experimental results.

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